

New York Scientific Data Summit 2020:

Data-Driven Discovery in Science and Industry

This conference will be held as an interactive virtual event
October 20–23, 2020



Note: All times are shown in EDT

Tuesday, October 20 - Climate

- 12:00 – 12:05 PM *Opening*, Meifeng Lin (Brookhaven National Laboratory)
- 12:05 – 12:10 PM *Welcome Remarks*, Kerstin Kleese van Dam (Director, Computational Science Initiative, Brookhaven National Laboratory)

Session #1, Session Chair: Nathan Urban (Brookhaven National Laboratory)

- 12:10 – 1:10 PM **Keynote:** *Climate, carbon, and water Tracking and anticipating human impacts*, Anna Michalak (Carnegie Institution for Science),
- 1:10 – 1:55 PM *Quantifying parameter uncertainty within a climate model*, Oliver Dunbar (California Institute of Technology)
- 1:55 – 2:00 PM *Virtual Coffee Break*

Session #2, Session Chair: Frank Alexander (Brookhaven National Laboratory)

- 2:00 – 2:30 PM Lightning Talk Session #1
- 2:30 – 3:15 PM *Numerical Methods for Predicting Coastal Flooding With Uncertainty*, Kyle Mandli (Columbia University),
- 3:15 – 4:15 PM **Panel Discussion - Challenges and Opportunities for Climate and Environmental Research**
- Moderator: Allison McComiskey (Brookhaven National Laboratory)
- Panelists: Anna Michalak (Carnegie Institution for Science), Oliver Dunbar (California Institute of Technology), Kyle Mandli (Columbia University)
- 4:15 – 5:00 PM *Virtual Social Hour via Zoom*

Wednesday, October 21 - Critical Infrastructure/Manufacturing

Session #3, Session Chair: TBD

- 12:00 – 1:00 PM **Keynote:** *Risk in power grids*, Daniel Bienstock (Columbia University)

1:00 – 1:45 PM *Cyber-Physical Systems for Smart Cities: a Mobility Perspective*, Desheng Zhang (Rutgers University),

1:45 – 2:00 PM *Virtual Coffee Break*

Session #4, Session Chair: Robert Harrison (Stony Brook University)

2:00 – 2:15 PM Lightning Talk Session #2

2:15 – 3:00 PM *Computational Modeling at GE*, Richard Arthur (General Electric Research),

3:00 – 4:00 PM **Panel Discussion - Challenges and Opportunities in Critical Infrastructure and Manufacturing**

Moderator: Karen Willcox (University of Texas – Austin)

Panelists: Daniel Bienstock (Columbia University), Desheng Zhang (Rutgers University), Richard Arthur (General Electric Research)

4:00 – 5:00 PM *Virtual Social Hour via Zoom*

Thursday, October 22 – Health and Medicine

Session #5, Session Chair: TBD

12:00 – 1:00 PM **Keynote: Re-Engineering the Future of Health with Predictive Models**, Grace C.Y. Peng (National Institutes of Health)

1:00 – 1:45 PM *Applications of AI in Cancer Research – Preparations, Progress and Predictions*, Eric Stahlberg (Frederick National Laboratory for Cancer Research)

1:45 – 2:00 PM *Virtual Coffee Break*

Session #6, Session Chair: Shantenu Jha (Rutgers University/Brookhaven National Laboratory)

2:00 – 2:15 PM Lightning Talk Session #3

2:15 – 3:00 PM *Data-driven modeling of COVID-19: Lessons Learned*, Ellen Kuhl (Stanford University)

3:00 – 3:45 PM *Computational Microscopy of SARS-CoV-2*, Rommie Amaro (University of California – San Diego)

3:45 – 4:00 PM *Virtual Coffee Break*

4:00 – 5:00 PM **Panel Discussion – Challenges and Opportunities in Computational Medicine/Health**

Moderator: Arvind Ramanathan (Argonne National Laboratory)

Panelists: Grace C.Y. Peng (NIH), Eric Stahlberg (Frederick National Laboratory for Cancer Research), Ellen Kuhl (Stanford University)

Friday, October 23 – Cross Cutting Topics

Session #7, Session Chair: Andrew Millis (Flatiron Institute)

- 12:00 – 1:00 PM **Keynote:** *Drug design and discovery for SARS-CoV2 by integrating artificial intelligence and physics-based models*, Arvind Ramanathan (Argonne National Laboratory)
- 1:00 – 1:45 PM *The quantum many-body problem as a challenge for machine learning methods*, Giuseppe Carleo (EPFL, Switzerland)
- 1:45 – 2:00 PM *Virtual Coffee Break*

Session #8, Session Chair: Qiang Du (Columbia University)

- 2:00 – 2:15 PM Lightning Talk Session #4
- 2:15 – 3:00 PM *The non-uniform FFT and its applications*, Leslie Greengard (New York University)
- 3:00 – 3:45 PM *HPC+AI: pushing molecular dynamics simulation with ab initio accuracy to 100 million atoms*, Lin Lin (University of California - Berkeley)
- 3:45 – 4:00 PM *Virtual Coffee Break*
- 4:00 – 5:00 pm **Concluding Discussions**
Moderator: Frank Alexander (Brookhaven National Laboratory)

October 20, 2020

2:00 - 2:30 PM, Lightning Talk Session #1

1. Artificial Intelligence for the Accuracy and Speed of Multiscale Modeling (Changnian Han, Peng Zhang, Jawaad Sheriff, Guojing Cong, Danny Bluestein, Yuefan Deng)
2. Exploring Sensitivity of ICF Outputs to Design Parameters in Experiments using Machine Learning (Julia Nakhleh, M. Giselle Fernández-Godino, Michael Grosskopf, Brandon Wilson, John Kline, Gowri Srinivasan)
3. Multitask Learning and Multi-Armed Bandit-Based Bayesian Optimization for High-Performance Computing Applications (Yang Liu, Xinran Zhu, Wissam M. Sid-Lakhdar, Osni A. Marques, Xiaoye S. Li, James W. Demmel)
4. Alzheimer's Disease Prognosis Using Graph Convolutional Neural Networks (Animesh Ghose, Shinjae Yoo, Ai Kagawa)
5. Examining graph topology using quantum walks (Raffaele Miceli, Michael McGuigan)

October 21, 2020

2:00 - 2:15 PM, Lightning Talk Session #2

1. Identifying Complex Physics Relationships using Sparse Matrix Decomposition to Inform Plasma Fusion Design (M. Giselle Fernández-Godino, Julia B. Nakhleh, Michael J. Grosskopf, Brandon M. Wilson, John Kline, Gowri Srinivasan)
2. Using Unstructured Data to Improve Homelessness and Suicide Prediction (Rafael Zamora-Resendiz, Destinee Morrow, Silvia Crivelli)
3. e3nn: 3D Euclidean symmetry equivariant neural networks -- Learning from the geometry and geometric tensors of physical systems (Tess E. Smidt, Mario Geiger, Benjamin Kurt Miller, Kostiantyn Lapchevskyi)

October 22, 2020

2:00 - 2:15 PM, Lightning Talk Session #3

1. Thermal Analysis of the SARS-CoV-2 Spike Glycoprotein by in silico and in vitro Experiments on the Supercomputers (Meichen Song, Fan Yang, Miriam Rafailovich, Marcia Simonc, Yuefan Deng, Peng Zhang)
2. Millisecond Multiscale Simulations of Multi-Platelet Aggregation in Shear Flow on Supercomputers (Yicong Zhu, Changnian Han, Peng Zhang, Guojing Cong, Danny Bluestein, Yuefan Deng)
3. AI Meets HPC: Learning the Platelet Dynamics from In Vitro and In Silico Experiments (Ziji Zhang, Changnian Han, Peng Zhang, Guojing Cong, Jawaad Sheriff, Danny Bluestein)

October 23, 2020 2:00 – 2:15 PM, Lightning Talk Session #4

1. The pH-varying Conformational States of SARS-CoV-2 Spike Glycoprotein (Ziyuan Niu, Yuefan Deng, Zhang Peng)
2. Simulating the Ground State Energies of Molecules Using IBM's Quantum Emulators (Mohammad Hassan, Michael McGuigan)
3. Quantum Computations of Dark Energy Models (Juan Varela, Michael McGuigan)